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A CLASS OF NONLINEAR MULTISTEP A-STABLE NUMERICAL METHODS FOR SOLVING STIFF DIFFERENTIAL EQUATIONS*

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Abstract—A family of nonlinear multistep (NLMS) methods is formulated to be A-stable in the sense of Dahlquist. These methods are a generalization of linear multistep methods and are particularly effective for solving differential equations whose solutions are asymptotically stable. NLMS methods have been applied to several 'stiff' differential equations whose solutions are illustrated. An analysis of step size choice is given.

1. INTRODUCTION

Classical numerical methods solve initial value problems of systems of first-order ordinary differential equations of the following type

$$y' = f(t, y); \quad y(t_0) = y_0. \tag{1}$$

If $\|\partial f/\partial y\|$ is large, a prohibitively small step size is required for accuracy if conventional numerical methods are used. To overcome this difficulty, we choose to express (1) in the form

$$y' = Ay + g(t, y); \quad y(t_0) = y_0. \tag{2}$$

where A is a constant matrix.

Frequently, 'stiff' differential equations occur in format (2) where $\mathrm{Re}\{\lambda(A)\} < 0$ and $\lambda(A)$, the eigenvalues of A, differ greatly in magnitude. These stiff equations occur in the applications to chemical kinetics, reactor kinetics, missile guidance, control theory, etc. It should be noted that the method given here works well even when $\mathrm{Re}\{\lambda(A)\} \geq 0$ [1]. In this paper a family of strongly stable nonlinear multistep (NLMS) methods that avoid using small step sizes are formulated.

NLMS methods are formulated to be consistent and selected to be strongly stable. As a consequence, NLMS methods are convergent (as proved in [1]). The consistency and strong stability will show up in the formulation. These methods are A-stable in the sense of Dahlquist [2] (shown in Section 2). NLMS methods are designed to avoid the use of small step sizes, and an illustration will be given in Section 3. The validity of NLMS methods is demonstrated by examples given in Section 5. These examples are solved by a package of FORTRAN programs, developed to implement NLMS methods, using the UNIVAC 1108 computer with double precision arithmetic. This package includes:

(1) a variable step size capability using predictor-corrector methods,
(2) self-starting features,
(3) an ability to handle $A(t)$, a time dependent matrix,
(4) Linear Multistep methods (LMS).

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A listing of this package in ANSI FORTRAN is available upon request directly from the authors. The complete theory of NLMS methods appears in [1].

2. FORMULATION

The linear multistep (LMS) methods of step k [5] can be expressed by

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i} \tag{3}$$

where $\alpha_k \neq 0$, $|\alpha_0| + |\beta_0| > 0$, α_i, β_i are scalar constants independent of mesh size h. LMS can solve (1) efficiently when $\|\partial f/\partial y\|$ is small. A natural generalization of (3) leads to the NLMS methods of step k in the form

$$\sum_{i=0}^{k} \alpha_i \, e^{Ah(k-i)} y_{n+i} = h \sum_{i=0}^{k} \phi_{ki}(Ah) g_{n+i} \tag{4}$$

where $\alpha_k \neq 0$, $|\alpha_0| + |\lambda(\phi_{k0}(Ah))| > 0$, and α_i are scalar constants independent of h, but $\phi_{ki}(Ah)$ are functions of h and nonsingular A. Note that this generalization leads to a formulation which depends nonlinearly on the mesh size h. As a consequence, we have labelled the method 'Nonlinear Multistep'. Others have called members of our family of methods as 'Exponential Methods' [3]. (The generalized Adams–Bashforth (GAB) and the generalized Adams–Moulton (GAM) methods for $k = 1, 2$ are suggested by Certaine [4]).

The NLMS methods are designed to solve (2) effectively when $\|\partial f/\partial y\| = \|A + (\partial g/\partial y)\|$ is large.

We begin by considering a homogeneous equation (2), i.e. $g(t, y) = 0$. Hence (2) can be written as

$$y' = Ay; \quad y(t_0) = y_0. \tag{2'}$$

The solution of (2') is

$$y(t) = e^{At} y(t_0).$$

Consequently,

$$y(t_{n+i}) = e^{iAh} y(t_n) \tag{5}$$

is the rigorous solution of (2') in the absence of round-off errors where $i = 0, 1, 2, \ldots$, an integer index and $h = t_{n+1} - t_n$. If (4) is to hold when $y(t_{n+i}) = e^{iAh} y(t_n)$, then substituting (5) into (4) gives

$$\sum_{i=0}^{k} \alpha_i \, e^{Ah(k-i)} e^{iAh} y(t_n) = e^{Ahk} y(t_n) \sum_{i=0}^{k} \alpha_i. \tag{6}$$

For $y(t_n) \neq 0$ and (6) to be zero, we discover that $\sum_{i=0}^{k} \alpha_i$ must be 0. This is identical to the first necessary condition for LMS to be consistent. The characteristic polynomial, following Henrici [5] and Dahlquist [2], for LMS methods is expressed by

$$\rho(\zeta) = \sum_{i=0}^{k} \alpha_i \zeta^i. \tag{7}$$

The above condition is recognized to give $\rho(1) = 0$. The stability of LMS methods is determined by examining the roots of $\rho(\zeta)$. Formula (6) can be written alternatively as

$$\sum_{i=0}^{k} \alpha_i \, e^{Ah(k-i)} (e^{Ah}\zeta)^i = e^{Ahk} \sum_{i=0}^{k} \alpha_i \zeta^i = e^{Ahk} \rho(\zeta) \tag{8}$$

which is seen to be proportional to $\rho(\zeta)$ of LMS methods. It is easily seen that (8) and (7) share

the same root condition. Later we shall describe that in order to simply determine $\phi_{ki}(Ah)$, we may select α_i. Therefore we may select strongly stable NLMS methods.

Dahlquist[2] defined a method to be A-stable if the numerical solution $\|y_n\| \to 0$ asymptotically as $n \to \infty$ for the differential equation $y' = Ay$ where $\mathrm{Re}\{\lambda(A)\} < 0$. A-stability is an important and desirable property when solving asymptotically stable stiff differential equations. When applying NLMS methods to the problem, $y' = Ay$ that is $g(t, y) = 0$, NLMS methods, in the absence of round-off errors, and errors of the exponential approximation, produce the solution to the problem, $y_n = e^{At_n} y_0 = e^{nAh} y_0$.

We calculate e^{nAh} by Pade approximation. For $\mathrm{Re}\{\lambda(A)\} < 0$, the Pade approximation is stable[6]. Thus it follows that $\lim_{n\to\infty} \|y_n\| \to 0$, establishing the A-stability in the sense of Dahlquist. The NLMS is best motivated by considering the first integral of (2), via an integrating factor, for A a constant matrix,

$$\frac{\mathrm{d}}{\mathrm{d}t}(e^{-At}y) = e^{-At}g(t, y); \quad y(t_0) = y_0. \tag{9}$$

Integration of (9) over the interval $[t_n, t_{n+i}]$ gives

$$y(t_{n+i}) = e^{iAh}y(t_n) + \int_{t_n}^{t_{n+i}} e^{A(t_{n+i}-t')}g(t', y)\,\mathrm{d}t'. \tag{10}$$

Expanding $g(t', y)$ by Taylor series expansion around t_n and substituting it into (10), we obtain

$$y(t_{n+i}) = e^{iAh}y(t_n) + \sum_{j=0}^{\infty} \frac{I_i^j(Ah)}{j!} g^{(j)}(t_n, y(t_n)), \tag{11}$$

where

$$I_i^j(Ah) = \int_{t_n}^{t_{n+i}} e^{A(t_{n+i}-t')}(t' - t_n)^j\,\mathrm{d}t'.$$

We define the nonlinear multistep operator

$$L[y(t); h] = \sum_{i=0}^{k} \alpha_i e^{Ah(k-i)} y(t + ih) - h \sum_{i=0}^{k} \phi_{ki}(Ah) g(t + ih, y(t + ih)). \tag{12}$$

Expanding $g(t + ih, y)$ in powers of h at $t = t_n$ yields

$$g(t + ih, y) = \sum_{j=0}^{\infty} \frac{(ih)^j}{j!} g^{(j)}(t_n, y(t_n)). \tag{13}$$

If we substitute (13) into (12), and use (11) for $y(t + ih)$ in (12), we obtain

$$\begin{aligned} L[y(t); h] &= \sum_{i=0}^{k} \alpha_i e^{Ah(k-i)} \left[e^{iAh} y + \sum_{j=0}^{\infty} \frac{I_i^j(Ah)}{j!} g^{(j)} \right] - h \sum_{i=0}^{k} \phi_{ki}(Ah) \left[\sum_{j=0}^{\infty} \frac{(ih)^j}{j!} g^{(j)} \right] \\ &= \left\{ \sum_{i=0}^{k} \alpha_i e^{Ah(k-i)} e^{iAh} y \right\} + \sum_{j=0}^{\infty} C_j(Ah) g^{(j)} \end{aligned} \tag{14}$$

where

$$C_j(Ah) = \sum_{i=0}^{k} \alpha_i e^{Ah(k-i)} \left[\frac{I_i^j(Ah)}{j!} \right] - h \sum_{i=0}^{k} \frac{(ih)^j}{j!} \phi_{ki}(Ah). \tag{15}$$

$\{\cdot\}$ of (14) $= e^{Ahk} \sum_{i=0}^{k} \alpha_i y$ vanishes because the first condition of consistency requires that the summation of α_i taken from $i = 0$–k equal 0. Therefore;

$$L[y(t); h] = \sum_{j=0}^{\infty} C_j(Ah) g^{(j)}. \tag{16}$$

Following Keller[7] a NLMS method of (4) is said to be consistent if

$$\max_n \left\| \sum_{i=0}^{k} \alpha_i \, e^{Ah(k-i)} y_{n+i} - h \sum_{i=0}^{k} \phi_{ki}(Ah) g_{n+i} \right\| \tag{17}$$

is small as $h \to 0$.

By induction, we can find that

$$\frac{A^{j+1} I_i^j(Ah)}{j!} = e^{iAh} - \sum_{l=0}^{j} \frac{(iAh)^l}{l!}.$$

Therefore, (15) becomes

$$-A^{j+1} C_j(Ah) = \sum_{i=0}^{k} \alpha_i \, e^{Ah(k-i)} \sum_{l=0}^{j} \frac{(iAh)^l}{l!} + \frac{(Ah)^{j+1}}{j!} \sum_{i=0}^{k} (i)^j \phi_{ki}(Ah). \tag{18}$$

For a p^{th}-order NLMS method, we require that $C_j(Ah) = 0$ for $j = 0, 1, \ldots, p$ but $C_{p+1}(Ah) \neq 0$.

The requirement, $C_j(Ah) = 0$, $j = 0, 1, \ldots, p$, satisfies consistency and permits formulating NLMS methods in the following matrix form, leading to the solution of ϕ when the α_i are selected so that NLMS methods are strongly stable.

$$E\psi = -HK\phi \tag{19}$$

where E, ψ, H, K and ϕ are described for both explicit and implicit methods. The expanded matrix forms for both explicit and implicit methods are described as follows.

Explicit: $\phi_{kk} \equiv 0$.

$$\begin{bmatrix} I & I & \cdots & I \\ I & I + Ah & \cdots & I + kAh \\ \vdots & \vdots & & \vdots \\ I & \sum_{m=0}^{p-1} \frac{(Ah)^m}{m!} & \cdots & \sum_{m=0}^{p-1} \frac{(kAh)^m}{m!} \end{bmatrix} \begin{bmatrix} \alpha_0 e^{kAh} \\ \alpha_1 e^{(k-1)Ah} \\ \vdots \\ \alpha_k I \end{bmatrix}$$

$$= - \begin{bmatrix} \frac{Ah}{0!} & & & \bigcirc \\ & \frac{(Ah)^2}{1!} & & \\ & & \ddots & \\ \bigcirc & & & \frac{(Ah)^p}{(p-1)!} \end{bmatrix} \begin{bmatrix} I & I & \cdots & I \\ 0 & I & \cdots & (k-1)I \\ \vdots & \vdots & & \vdots \\ 0 & I & \cdots & (k-1)^{p-1} I \end{bmatrix} \begin{bmatrix} \phi_{k0} \\ \phi_{k1} \\ \vdots \\ \phi_{k,k-1} \end{bmatrix}$$

Implicit: $\phi_{kk} \neq 0$

$$\begin{bmatrix} I & I & \cdots & I \\ I & I + Ah & \cdots & I + kAh \\ \vdots & \vdots & & \vdots \\ I & \sum_{m=0}^{p} \frac{(Ah)^m}{m!} & \cdots & \sum_{m=0}^{p} \frac{(kAh)^m}{m!} \end{bmatrix} \begin{bmatrix} \alpha_0 e^{kAh} \\ \alpha_1 e^{(k-1)Ah} \\ \vdots \\ \alpha_k I \end{bmatrix}$$

$$= - \begin{bmatrix} \frac{Ah}{0!} & & & \bigcirc \\ & \frac{(Ah)^2}{1!} & & \\ & & \ddots & \\ \bigcirc & & & \frac{(Ah)^{p+1}}{p!} \end{bmatrix} \begin{bmatrix} I & I & \cdots & I \\ 0 & I & \cdots & kI \\ \vdots & \vdots & & \vdots \\ 0 & I & \cdots & k^p I \end{bmatrix} \begin{bmatrix} \phi_{k0} \\ \phi_{k1} \\ \\ \phi_{kk} \end{bmatrix}$$

We determine $\phi_{ki}(Ah)$, without loss of generality, by selecting $\alpha_k = 1$ and then, requiring that the condition of strong stability be realized in selecting α_i's. If we select $\alpha_k = 1$, $\alpha_{k-1} = -1$, and $\alpha_{k-2} = \alpha_{k-3} = \cdots = \alpha_0 = 0$, then we arrive at what we have called the Generalized Adams methods. The $\phi_{ki}(Ah)$ are determined utilizing the above matrix formula, which can be considered as a matrix equation for the k-step, p^{th}-order method ($k \geq 1$, $p \geq 1$). Below we show that $\phi_{ki}(Ah)$ can be determined by listing the formula for the remaining $\phi_{ki}(Ah)$'s. From (19) for nonsingular H and K, we get

$$\phi = -K^{-1}H^{-1}E\psi, \tag{20}$$

where ϕ is a vector of dimension $(k-1)$ or k depending upon whether the scheme is explicit or implicit.

Explicit schemes

$k = p = 1$,

$$\phi_{1,0}(Ah) = -(Ah)^{-1}(\alpha_0 e^{Ah} + I).$$

$k = p = 2$,

$$\phi_{2,0}(Ah) = -(Ah)^{-2}(\alpha_0(Ah - I)e^{2Ah} - \alpha_1 e^{Ah} - (I + Ah)).$$

$$\phi_{2,1}(Ah) = -(Ah)^{-2}(\alpha_0 e^{2Ah} + \alpha_1(I + Ah)e^{Ah} + (I + 2Ah)).$$

$k = p = 3$,

$$\phi_{3,0}(Ah) = -(Ah)^{-3}[\alpha_0(I - 3Ah/2 + (Ah)^2)e^{3Ah} + \alpha_1(I - Ah/2)e^{2Ah} + \alpha_2(I + Ah/2)e^{Ah} + I + 3Ah/2 + (Ah)^2].$$

$$\phi_{3,1}(Ah) = -(Ah)^{-3}[-2\alpha_0(I - Ah)e^{3Ah} + \alpha_1(-2I + (Ah)^2)e^{2Ah} - 2\alpha_2(I + Ah)e^{Ah} - (2I + 4Ah + 3(Ah)^2)].$$

$$\phi_{3,2}(Ah) = -(Ah)^{-3}[\alpha_0(I - Ah/2)e^{3Ah} + \alpha_1(I + Ah/2)e^{2Ah} + \alpha_2(I + 3Ah/2 + (Ah)^2)e^{Ah} + (I + 5Ah/2 + 3(Ah)^2)].$$

Implicit schemes

$k = p = 1$,

$$\phi_{1,0}(Ah) = -(Ah)^{-2}(\alpha_0(Ah - I)e^{Ah} - I).$$

$$\phi_{1,1}(Ah) = -(Ah)^{-2}(\alpha_0 e^{Ah} + (I + Ah)).$$

$k = p = 2$,

$$\phi_{2,0}(Ah) = -(Ah)^{-3}[\alpha_0(I - 3Ah/2 + (Ah)^2)e^{2Ah} + \alpha_1(I - Ah/2)e^{Ah} + (I + Ah/2)].$$

$$\phi_{2,1}(Ah) = -(Ah)^{-3}[\alpha_0(-2I + 2Ah)e^{2Ah} + \alpha_1(-2I + (Ah)^2)e^{Ah} - 2(I + Ah)].$$

$$\phi_{2,2}(Ah) = -(Ah)^{-3}[\alpha_0(I - Ah/2)e^{2Ah} + \alpha_1(I + Ah/2)e^{Ah} + (I + 3Ah/2 + (Ah)^2)].$$

$k = p = 3$,

$$\phi_{3,0}(Ah) = -(Ah)^{-4}[\alpha_0(-I + 2Ah - 11(Ah)^2/6 + (Ah)^3)e^{3Ah} + \alpha_1(-I + Ah - (Ah)^2/3)e^{2Ah} + \alpha_2(-I + (Ah)^2/6)e^{Ah} + (-I - Ah - (Ah)^2/3)].$$

$$\phi_{3,1}(Ah) = -(Ah)^{-4}[\alpha_0(3I - 5Ah + 3(Ah)^2)e^{3Ah} + \alpha_1(3I - 2Ah - (Ah)^2/2 + (Ah)^3)e^{2Ah} + \alpha_2(3I + Ah - (Ah)^2)e^{Ah} + (3I + 4Ah + 3(Ah)^2/2)].$$

$$\phi_{3,2}(Ah) = -(Ah)^{-4}[\alpha_0(-3I + 4Ah - 3(Ah)^2/2)e^{3Ah} + \alpha_1(-3I + Ah + (Ah)^2)e^{2Ah} + \alpha_2(-3I - 2Ah + (Ah)^2/2 + (Ah)^3)e^{Ah} + (-3I - 5Ah - 3(Ah)^2)].$$

$$\phi_{3,3}(Ah) = -(Ah)^{-4}[\alpha_0(I - Ah + (Ah)^2/3)e^{3Ah} + \alpha_1(I - (Ah)^2/6)e^{2Ah} + \alpha_2(I + Ah + (Ah)^2/3)e^{Ah} + (I + 2Ah + 11(Ah)^2/6 + (Ah)^3)].$$

3. SELECTION OF STEP SIZE

Conventionally, when using LMS k-step methods with $\alpha_k = 1$, we select h such that

$$\beta_k h L^* \sim \mu \ (<1).$$

Similarly for NLMS methods, we select h_N to satisfy

$$\|\phi_{kk}(Ah_N)\| h_N L \sim \mu \ (<1).$$

If we combine them together, we see that $h_N = \|\phi_{kk}^{-1}(Ah_N)\|\beta_k(L^*/L)h$. For $\|\phi_{kk}^{-1}(Ah_N)\|\beta_k$ not too small, we know that $L^* \gg L$; therefore $h_N \gg h$, where L^* and L are $\|\partial f/\partial y\|$ and $\|\partial g/\partial y\|$ respectively. In the case, $g(t, y)$ is independent of y, and slowly varying with t, NLMS permits the use of a large step size. In practice, one may be further constrained by the approximation of e^{Ah}.

Let us consider the following example:

$$y' = -100y + (1 + t^2); \quad y(0) = 1; \quad t \in [0, 100].$$

Using LMS methods for $k = 3$, we select h such that

$$\beta_k h(100) < 1 \rightarrow h < 0.027.$$

Using NLMS methods of $k = 3$ we select h_N such that

$$\|\phi_{kk}(Ah_N)\| \cdot h_N \cdot \left\|\frac{\partial g}{\partial y}\right\| < 1.$$

Since $\|\partial g/\partial y\| = 0$ we can select h_N of any size. In the results below, we arbitrarily choose $h_N = 25$ and record the solutions at $t = 100$. This method can reach $t = 100$ in one step, whereas conventional LMS methods would require ~25,000 steps for equivalent accuracy.

Methods	h	Solution
LMS	2^{-8}	0.9999 0002E+02
NLMS	25	0.9999 0002E+02
Exact		0.9999 0002E+02

4. IMPLEMENTATION OF NLMS METHODS

A package of computer programs was originally designed using the FORTRAN language to implement NLMS methods on the UNIVAC 1108 computer. The same package was made operational on the IBM 360 and CDC 6600 computers in ANSI FORTRAN language. There are a number of useful features incorporated into the package; namely, variable step size, self-starting, selection of characteristic polynomial coefficients, A is a function of t, predict-and-correct-m-times, and the inclusion of linear multistep (LMS) methods. Detailed descriptions of this computer package have been documented in [8], copies of this reference can be obtained directly from the authors upon request.

5. APPLICATIONS

5.1 *A reactor kinetics problem* [9]

The infinite-medium reactor kinetic equations, in standard form, with m delayed neutron groups can be expressed as

$$\frac{dn}{dt} = -\frac{\delta K - \beta}{l} n + \sum_{i=1}^{m} \lambda_i C_i; \quad i = 1, \ldots, m \ \frac{dC_i}{dt} = \frac{\beta_i}{l} n - \lambda_i C_i$$

where β_i = the fraction of the total number of fission neutrons belonging to the i^{th} group precursor which are delayed; β = the fraction of the fission neutron which are delayed; l = neutron generation time (s); λ_i = decay constant for the i^{th} group precursor; n = neutron density; C_i = the concentration of the i^{th} precursor; and δK = a constant for a reactor with a constant excess of reactivity.

Consider a single delayed neutron group, we have

$$\begin{bmatrix} \frac{dn}{dt} \\ \frac{dC_1}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{\delta K - \beta}{l} & \lambda_1 \\ \frac{\beta_1}{l} & -\lambda_1 \end{bmatrix} \begin{bmatrix} n \\ C_1 \end{bmatrix}$$

Using the initial condition, $(n(0), C_1(0))^T = (1, -1)^T$, and the input values

$$\beta = 0.0075; \qquad \lambda_1 = 0.075; \qquad l = 10^{-6};$$
$$\beta_1 = 0.0075; \qquad \delta K = 1.0075;$$

the exact solution vector, $y(t) = (n(t), C_1(t))^T$, has the values

$$y(2) = (-0.64141073 - 07, -0.85521424 - 00)^T,$$
$$y(5) = (-0.51304190 - 07, -0.68405581 - 00)^T,$$
$$y(10) = (-0.35360130 - 07, -0.47146837 - 00)^T.$$

We note that this system is extremely stiff since the eigenvalues of A are -10^6 and -0.0744375.

Using fixed-step-size ($h = 1$), explicit NLM-1-step method, numerical results show:

t	$n(t)$	$C_1(t)$	Solution
2	−0.64141073 − 07	−0.85521424 − 00	NILMS
	−0.64141073 − 07	−0.85521424 − 00	Exact
5	−0.51304190 − 07	−0.68405581 − 00	NLMS
	−0.51304190 − 07	−0.68405581 − 00	Exact
10	−0.35360130 − 07	−0.47146837 − 00	NLMS
	−0.35360130 − 07	−0.47146837 − 00	Exact

5.2 *A stiff system*

The following example was proposed by Krogh [10] and solved by stiffly stable methods [11]. This test example is not well-posed in the large; errors greater than 10^{-3} near equilibrium can cause the perturbed solution to be unbounded. An explicit NLM-1-step method was used with a fixed step size $h = 10^{-3}$ for $t < 1$ and $h = 10^{-2}$ for $1 \leq t \leq 10$ and $h = 0.1$ for $t > 10$. We tabulate our experimental results at the same step sizes that Gear used.

$$\text{Problem:} \quad y' = Uz - UBUy; \quad y(0) = (-1, -1, -1, -1)^T$$

where

$$U = \frac{1}{2}\begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix};$$

$$z = (w_1^2, w_2^2, w_3^2, w_4^2)^T = Uy;$$

and

$$B = \text{diag}\,(\beta_1, \beta_2, \beta_3, \beta_4);$$

$$\beta_1 = 1000, \quad \beta_2 = 800, \quad \beta_3 = -10, \quad \beta_4 = 0.001.$$

The exact solution is: $y(t) = U(s_1, s_2, s_3, s_4)^T$;

$$s_i = \frac{\beta_i}{1 - (1 + \beta_i)\, e^{\beta_i t}}, \quad i = 1, 2, 3, 4.$$

Numerical results show:

Current time t	Max step size	Matrix inversions	Max error
1	10^{-3}	1	0.5010D-4
10	10^{-2}	2	0.1475D-4
100	10^{-1}	3	0.2302D-5
500	10^{-1}	3	0.1628D-6
1000	10^{-1}	3	0.7011D-7

Since only 3 different step sizes are used, it is to be noted that a total of 3 matrix inversions and 3 matrix exponentials are needed. To reach $t = 1000$ NLMS required 1.09×10^6 steps whereas Gear[11] indicates it would have taken 1.5×10^6 steps.

6. CONCLUSIONS

Numerical results show the effectiveness and the validity of NLMS methods for solving initial value problems of stiff equations of the form $y' = Ay + g(t, y)$.

When A is a function of t, the following approach may be used. Decompose

$$y' = A(t)y + g(t, y)$$

such that

$$y' = A(t_i)y + \{A(t) - A(t_i)\}y + g(t, y)$$

so the NLMS methods can be applied. Since above equation is stiff, $\mathrm{Re}\{\lambda(A(t))\} < 0$ for all t. If $\|A(t) - A(t_i)\|$ can be maintained small enough, the above problem can be solved accurately.

To illustrate the above approach, we consider

$$y' = t(1 - y) + (1 - t)\,e^{-t}; \quad y(0) = 1$$

which can be rewritten as

$$y' = -ty + \{t + (1 - t)\,e^{-t}\}; \quad y(0) = 1.$$

The exact solution is given by $y = e^{-t^2/2} - e^{-t} + 1$. Evidently, the A matrix reduces to a scalar function of t and the $g(t, y)$ after the decomposition becomes $\{t + (1 - t)\,e^{-t}\}$. This problem is a severe test of a method's ability to handle equations that cause stability problems[10]. Using variable-step-size NLM-3-step methods with initial $h = 0.01$ and h_{max} is set equal to 0.1 gives the following results.

t	$y(t)$
0.10000000+01	0.12386512−01*
	0.12386512−01†
0.10000000+02	0.99995460+00
	0.99995460+00
0.50005000+02	0.10000000+01
	0.10000000+01

*Produced by NLM-3-step methods.
†Exact solution.

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